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An explicit four-step phase-fitted method for the numerical integration of second-order initial-value problems

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Abstract

An explicit four-step method with phase-lag of infinite order is developed for the numerical integration of second-order initial-value problems. Extensive numerical testing indicates that this new method can be generally more efficient than other four-step methods.

Keywords: Second-order periodic initial-value problem; Phase-lag

1. Introduction

In recent years there has been considerable interest in the numerical solution of the initial-value problems of the form

$$y''(x) = f(x, y), \qquad y(x_0) = y_0 \quad \text{and} \quad y'(x_0) = y'_0 \tag{1.1}$$

involving ordinary differential equations of second order in which the derivative does not appear explicitly. Equations having oscillatory solutions are of particular interest. Examples occur in celestial mechanics, in quantum mechanical scattering problems, and elsewhere.

Recently, several methods with minimal phase-lag, a concept introduced in [1], have been proposed for the numerical integration of the initial-value problem (1.1). Chawla and Rao [3–6] have developed methods with phase-lag of order six and eight. Also, Thomas [14] has given a two-step sixth-order method with phase-lag of order eight. Van der Houwen and Sommeijer [15] have derived some four-step methods with minimal phase-lag. Coleman [7] has given a new approach to construct methods for the numerical integration of $y'' = f(x, y)$ via rational approximation for the cosine. Van der Houwen et al. [16] have proposed some methods with phase-lag of

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infinite order in some cases. Simos and Raptis [13] have derived some P-stable Numerov-type methods with phase-lag of order 8 and 10. Also, Raptis and Simos [12] have derived an implicit four-step method with phase-lag of infinite order. The purpose of this paper is to develop an explicit four-step method with phase-lag of order ∞, and with interval of periodicity $(0, 4.40831979^2)$. The idea is to maintain a free parameter in the method such that the method can be fitted to an oscillatory component of the theoretical solution, similar to the exponential fitting proposed by Liniger and Willoughby [10] and van der Houwen et al. for the solution of first-order equations.

Numerical results presented in Section 3 show that this new method is more accurate (especially for large step-sizes) than other four-step methods with minimal phase-lag.

2. Derivation of the phase-fitted method

For the numerical integration of the initial-value problem (1.1) consider the one-parameter family of four-step methods, which is denoted as $\mathrm{METH}_6(a)$:

$$\bar{y}_{n+2} = 2y_{n+1} - 2y_n + 2y_{n-1} - y_{n-2} + h^2/6(7(f_{n+1} + f_{n-1}) - 2f_n), \tag{2.1}$$

$$\bar{y}_n = y_n - ah^2(\bar{f}_{n+2} - 4f_{n+1} + 6f_n - 4f_{n-1} + f_{n-2}), \tag{2.2}$$

$$y_{n+2} - 2y_{n+1} + 2y_n - 2y_{n-1} + y_{n-2} = h^2/120[9(\bar{f}_{n+2} + f_{n-2}) + 104(f_{n+1} + f_{n-1}) + 14\bar{f}_n], \tag{2.3}$$

where $\bar{f}_{n+2} = f(x_{n+2}, \bar{y}_{n+2})$, $\bar{f}_n = f(x_n, \bar{y}_n)$ and a is a free parameter. The local truncation error is

$$\mathrm{LTE} = [-19/6048\, y_n^{(8)} - 1/4800(27 + 560a)F_n y_n^{(6)}]h^8 + \mathrm{O}(h^{10}), \tag{2.4}$$

where $F_n = (\partial f/\partial y)\,(x_n, y(x_n))$ and thus the method is of order 6 in general.

We apply these methods to the test equation $y'' = -k^2 y$. Setting $H = kh$ we obtain the stability polynomial:

$$P(w) = A(H)w^4 + B(H)w^3 + C(H)w^2 + B(H)w + A(H), \tag{2.5}$$

where $A(H) = 1$, $B(H) = -2 + 61/60\,H^2 - 7/240\,H^4\,(3 + 8a) - 49/360\,H^6 a$ and

$$C(H) = 2 - H^2/30 + H^4/120(3 + 56a) + 7/180\,H^6 a \tag{2.6}$$

Substituting in (2.5) $w = (1 + z)/(1 - z)$ we have

$$(1 - z)^4 P(w) = [2A(H) - 2B(H) + C(H)]z^4 + 2[6A(H) - C(H)]z^2 + 2A(H) + B(H) + C(H). \tag{2.7}$$

From (2.7) we have the polynomials:

$$P_1(H) = 2A(H) - 2B(H) + C(H) = 8 - 31/15\,H^2 + H^4(3 + 14a)/15 + 14/45\,H^6 a,$$

$$P_2(H) = 12A(H) - 2C(H) = 8 + H^2/15 - H^4/60(3 + 56a) - 7/90\,aH^6$$

and

$$P_3(H) = 2A(H) + 2B(H) + C(H) = 2H^2 - 3/20\,H^4 - 7/30\,H^6 a. \tag{2.8}$$

Definition 2.1. The method (2.1)–(2.3) is said to have *interval of periodicity* $(0, H_0^2)$ if, for all $H^2 \in (0, H_0^2)$, the roots w_i, $i = 1, 2, 3, 4$, of (2.5) satisfy

$$w_1 = e^{iu(H)}, \quad w_2 = e^{-iu(H)} \quad \text{and} \quad |w_t| \leqslant 1, \quad t = 3, 4, \tag{2.9}$$

where $u(H)$ is a real function of H.

It is obvious that if $w \neq 0$ is a root in $P(w)$ in (2.5) so is w^{-1}. Hence, we have that all the roots of $P(w)$ must have modulus equal to 1. So, we have the next lemma.

Lemma 2.2 (Raptis and Simos [12]). *All the four-step methods with the stability polynomial given by* (2.7) *have interval of periodicity* $(0, H_0^2)$ *if*

$$\begin{aligned} &P_1(H), P_2(H), P_3(H) \geqslant 0, \\ &S(H) = P_2(H)^2 - 4P_1(H)P_3(H) \geqslant 0. \end{aligned} \tag{2.10}$$

for all $H^2 \in (0, H_0^2)$.

For the four-step methods which have the stability polynomial given by (2.5) and (2.6) we have the next lemma.

Lemma 2.3 (Raptis and Simos [12]). *For all H in the interval of periodicity, the phase-lag of the four-step method with stability polynomial given by* (2.5) *and* (2.6) *is* $O(H^Q)$ *if*

$$\frac{2A(H)\cos(2H) + 2B(H)\cos(H) + C(H)}{H[4A(H)\sin(2H) + 2B(H)\sin(H)]} = O(H^Q) \tag{2.11}$$

and we say that the phase-lag of the method is of order Q if (2.11) is valid.

Definition 2.4. We call a method *phase-fitted* if it has phase-lag of order ∞.

Theorem 2.5. *The method* (2.1)–(2.3) *has a phase-lag of infinite order if*

$$a = \frac{12H^2[1 + 61\cos(H)] - 720[1 - 2\cos(H) + \cos(2H)] - 9H^4[1 - 7\cos(H)]}{168H^4[1 - \cos(H)] + 14H^6[1 - 7\cos(H)]}. \tag{2.12}$$

In this case the interval of periodicity is $(0, 4.40831979^2)$.

Proof. To have a phase-lag of infinite order, it follows from (2.11) that

$$2A(H)\cos(2H) + 2B(H)\cos(H) + C(H) = 0. \tag{2.13}$$

With the help of (2.6) we have that the parameter a is given by (2.12).

For $H = 0$, we have $a = -751/35280$, whereas a is undefined for H such that the denominator of (2.12) $= 0$. Hence, one should avoid step-sizes h for which $H = hk$ are close to denominator $= 0$.

The explicit form of the coefficient a is given by

$$a = -751/35280 + 1529H^2/4233600 - 532121H^4/117355392000 + 2377667H^6/183074411520000 - 422600153H^8/461347517030400000.$$

Now if we substitute (2.12) into (2.8) we have

$$P_1(H) = \frac{16[(H^2+3)\cos(2H) + 3H^2\cos(H) + 2H^2 - 3]}{(7H^2+12)\cos(H) - (H^2+12)},$$

$$P_2(H) = -\frac{4(H^2+12)[\cos(2H) - 4\cos(H) + 3]}{(7H^2+12)\cos(H) - (H^2+12)} \tag{2.14}$$

and

$$P_3(H) = -\frac{12H^2[\cos(2H) - 4\cos(H) + 3]}{(7H^2+12)\cos(H) - (H^2+12)}.$$

Based on Lemma 2.2 and from (2.8) and (2.14) we have $P_1(H) > 0$ for all $H \in (0, 4.40831979^2)$, $P_2(H) > 0$ for all $H \in (0, 6.28332520^2)$ and $P_3(H) > 0$ for all $H \in (0, 6.28338623^2)$.

So the interval of periodicity of this method is $(0, 4.40831979^2)$. □

3. Numerical illustrations

We illustrate the new method proposed in this paper by considering the following four examples. The first is the "almost periodic" problem studied by Franco and Palacios [9], the second is a nonlinear example, the third is an inhomogeneous equation and the last is the resonance problem of Schrödinger.

3.1. Problem 1

We consider the following "almost periodic" problem situated by Franco and Palacios [9]:

$$z'' + z = \varepsilon e^{i\varphi x}, \quad z(0) = 1, \; z'(0) = i, \; z \in \mathbb{C}, \tag{3.1}$$

whose theoretical solution is

$$z(x) = u(x) + iv(x), \quad u, v \in \mathbb{R},$$

$$u(x) = \frac{1 - \varepsilon - \varphi^2}{1 - \varphi^2}\cos(x) + \frac{\varepsilon}{1 - \varphi^2}\cos(\varphi x), \tag{3.2}$$

$$v(x) = \frac{1 - \varepsilon\varphi - \varphi^2}{1 - \varphi^2}\sin(x) + \frac{\varepsilon}{1 - \varphi^2}\sin(\varphi x).$$

The solution (3.2) represents motion on a perturbation of a circular orbit in the complex plane. We have written this problem as a coupled set of real differential equations for $u(x)$ and $v(x)$.

Table 1
Comparison of the absolute errors in the approximations obtained by methods 1–3 for $z(40\pi)$

h	Method 1	Method 2	Method 3
$\pi/2$	0.352×10^{-3}	0.562×10^{-1}	0.209×10^{-14}
$\pi/3$	0.608×10^{-3}	0.820×10^{-7}	0.333×10^{-15}
$\pi/4$	0.592×10^{-3}	0.513×10^{-8}	0.123×10^{-16}
$\pi/5$	0.278×10^{-3}	0.224×10^{-9}	0.000×10^{0}

This real system has been solved numerically for $0 \leqslant x \leqslant 40\pi$, $\varepsilon = 0.001$ and $\varphi = 0.01$, using exact starting values and the following methods:

Method 1: Predictor–corrector method of van der Houwen and Sommeijer [16, Eqs. (4.2a + b)].

Method 2: Four-step three-stage method of van der Houwen and Sommeijer [15, Eq. (4.7)].

Method 3: Explicit four-step phase-fitted method developed in this paper, where H is set to the step-size h.

The results are given in Table 1, with step-sizes presented in the first column, in which the error between the exact solution and the numerical solution in the form $\|z(x) - z_n\|_2$ is presented. On comparing these results, we see that for this problem and these step-sizes Method 3 is more accurate than any of the other methods, especially for large step-sizes.

3.2. *Problem 2: A nonlinear example*

As a second example, we consider Duffing's equation, forced by a harmonic function [17]:

$$y''(x) + y(x) + y^3(x) = c\cos(\varphi x), \quad t \in [0, X], \tag{3.3}$$

with parameter values $c = 0.002$ and $\varphi = 1.01$. The initial conditions are

$$y(0) = A, \quad y'(0) = 0, \tag{3.4}$$

where A is obtained from the Galerkin approximation y_G, evaluated at $x = 0$:

$$y_G(x) = \sum_{i=0}^{\infty} a_{2i+1}\cos[(2i+1)\varphi x]. \tag{3.5}$$

Van Dooren [17] calculated an approximation of order 9, having the same frequency as the forcing term; with an absolute precision of 10^{-12}, the coefficients are given by

$$a_1 = 0.200179477536, \quad a_3 = 0.246946143\times10^{-3}, \quad a_5 = 0.304014\times10^{-6},$$
$$a_7 = 0.374\times10^{-9}, \quad a_9 = 0. \tag{3.6}$$

Table 2 gives the absolute errors in $y(x)$ at $x = 24\pi$, with step-sizes shown in column 1 for the same methods as in Section 3.1. From this table we can see that again Method 3 gives the best results compared with other methods.

Table 2
Comparison of the absolute errors in the approximations obtained by methods 1–3 for $y(24\pi)$

h	Method 1	Method 2	Method 3
$2\pi/5$	0.184×10^{-2}	0.457×10^{-2}	0.289×10^{-4}
$\pi/5$	0.303×10^{-3}	0.118×10^{-3}	0.738×10^{-5}
$\pi/10$	0.304×10^{-4}	0.165×10^{-5}	0.130×10^{-6}

3.3. *Problem 3: Inhomogeneous equation*

We consider the equation

$$y'' = -\varphi^2 y + (\varphi^2 - 1)\sin(x), \quad x \geqslant 0, \tag{3.7}$$

with exact solution

$$y(x) = \cos(\varphi x) + \sin(\varphi x) + \sin(x), \quad \varphi \gg 1. \tag{3.8}$$

This is an inhomogeneous equation, whose exact solution consists of a rapidly and slowly oscillating function. The slowly varying function is due to the inhomogeneous term. The purpose is to show that the phase-fitted methods are able to integrate this problem with relatively large integration steps (i.e., h not small), because the high-order phase-lag will take care of the rapidly oscillating component and the algebraic order will take care of the slowly varying component. In our numerical example we take $\varphi = 10$.

Table 3 gives the absolute errors in $y(x)$ at $x = 30$, with step-sizes given in the first column, for the same three methods.

From these results we can see again that the explicit phase-fitted method gives much more accurate results compared with the other explicit methods.

3.4. *Problem 4*

The radial or one-dimensional Schrödinger equation may be written as

$$y''(x) = f(x)y(x), \qquad x \in [0, \infty), \tag{3.9}$$

Table 3
Comparison of the absolute errors in the approximations obtained by methods 1–3 for $y(30)$

h	Method 1	Method 2	Method 3
0.2	0.142×10^{-4}	0.142×10^{0}	0.281×10^{-6}
0.1	0.394×10^{-6}	0.750×10^{-4}	0.786×10^{-9}
0.05	0.220×10^{-7}	0.437×10^{-7}	0.209×10^{-10}

where $f(x) = W(x) - E$, and $W(x) = l(l+1)/x^2 + V(x)$ is an effective potential with $W(x) \to 0$ as $x \to \infty$, l is an integer, and E is a real number denoting the energy.

The problem is one of the boundary-value type, with $y(0) = 0$, and a second boundary condition for large values of x determined by physical considerations. We distinguish two types of the second boundary condition.

(i) If $E = \varphi^2 > 0$, then, in general, the potential function $V(x)$ dies away faster than the term $l(l+1)/x^2$; Eq. (3.9) then effectively reduces to $y''(x) + (E - l(l+1)/x^2)y(x) = 0$, for x greater than some value R depending on the potential function $V(x)$. The above equation has linearly independent solutions $\varphi x j_l(\varphi x)$ and $\varphi x n_l(\varphi x)$, where $j_l(\varphi x)$ and $n_l(\varphi x)$ are the spherical Bessel and Newmann functions respectively. Thus the solution of Eq. (3.9) has the asymptotic form

$$y(x) \underset{x\to\infty}{\cong} A\varphi x j_l(\varphi x) - B\varphi x n_l(\varphi x)$$

$$\underset{x\to\infty}{\cong} C[\sin(\varphi x - l\pi/2) + \tan\delta_1 \cos(\varphi x - l\pi/2)],$$

where δ_1 is the *phase shift* which may be calculated from the formula

$$\tan\delta_1 = [y(x_2)S(x_1) - y(x_1)S(x_2)]/[y(x_1)C(x_2) - y(x_2)C(x_1)]$$

for x_1 and x_2 distinct points on the asymptotic region with $S(x) = \varphi x j_l(\varphi x)$ and $C(x) = -\varphi x n_l(\varphi x)$.

Since the problem is treated as an initial-value problem, one needs y_0, y_1, y_2 and y_3 before starting a four-step method. From the initial condition, $y_0 = 0$. We know that for values of x close to the origin, the solution behaves as $y(x) = cx^{l+1}$. From this we determine $y_1 = h^{l+1}$. To calculate y_2 and y_3 we use the exponentially fitted method of Raptis [11]. With these starting values we evaluate at some point of the asymptotic region the phase shift δ_1 and the normalization factor C from the above relations.

(ii) If $E = -\varphi^2 < 0$, then the problem is an eigenvalue one, and can be solved by well-known techniques (see, for example, [2]). The solution decays exponentially for large values of x, $y(x) \cong \exp(-\sqrt{-E}x)$. The boundary value problem is split into two initial-value problems. Using a trial eigenvalue, one integrates forwards from the origin, and backwards from large values of x, and attempts to match the solution at some internal point. An iterative process then uses the degree of mismatch to calculate a correction of the eigenvalue [8].

In our numerical example we have used the Woods–Saxon with $l = 0$ potential i.e.,

$$W(x) = V(x) = u_0/(1+t) - (u_0/a)t/(1+t)^2,$$

where $t = \exp[(x - x_0)/a)$ and $u_0 = -50.0$, $a = 0.6$, $x_0 = 7.0$ and $x \in [0, \infty)$. We consider, in particular, the resonance problem for $E \in [1, 1000]$ with boundary conditions $y(0) = 0$ and $y(x) \cong \sin(\sqrt{E}x + \delta)$ at large values of x.

The resonance problem consists in finding values E_j of E (eigenenergies) at which the phase shift $\delta(E_j)$ equals $\pi/2$.

In our numerical test we shall use, for convenience, the exact eigenenergies E_j with six decimal digits accuracy, and an estimate of the phase in order to determine H and thus the free parameter a in our method. We put $H = \sqrt{E_j}h$, and successively compute the phase-shifts by the four

Table 4
Deviations of the computed phase-shifts from the exact value $\pi/2$, in 10^{-6} units for various choices of step-size shown in the second column. The empty areas indicate that the corresponding variations are larger than the format allowed in the table

E	h	Method 1	Method 2	Method 3
53.588872	1/8	126121	8578	74
	1/16	6698	22	0
	1/32	405	0	0
	1/64	25	0	0
163.215341	1/8	—	—	864
	1/16	21326	222	1
	1/32	1235	1	1
	1/64	76	0	0
341.495874	1/8	—	—	149024
	1/16	59154	1460	10
	1/32	3170	7	0
	1/64	192	0	0
989.701916	1/8	—	—	543289
	1/16	400726	213334	4060
	1/32	15071	20	1
	1/64	852	1	0

techniques denoted in Section 3.1. The deviations of the computed phase-shifts from the exact value $\pi/2$ are presented in Table 4.

From the results obtained we conclude that the new method is more accurate than the other methods, especially in cases of large step-sizes.

All computations were carried out on an IBM PC-AT 80386 with 80387 mathcoprocessor of the Informatics Laboratory, Agricultural University of Athens, using double-precision arithmetic with 14-digits accuracy.

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